Hydrogen and Methane Loaded Materials for Mitigation of GCRs and SPEs

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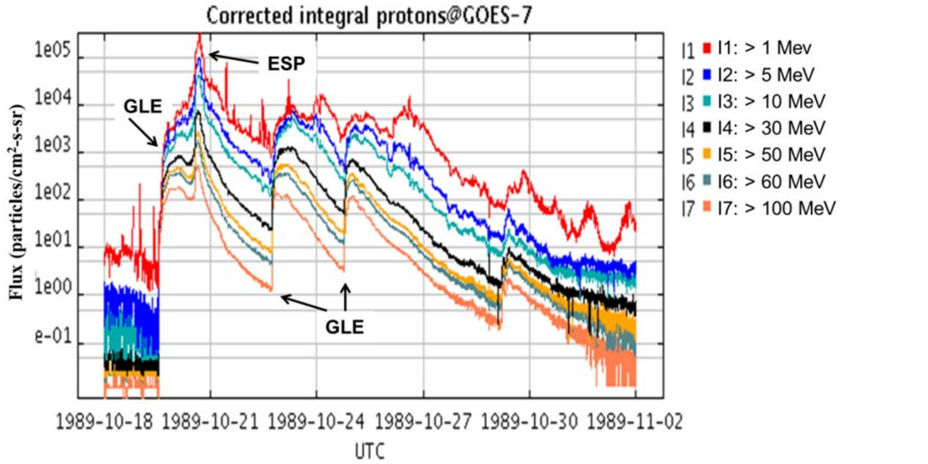
Outline

- Introduction
- Previous Work
- Hydrogen-loaded GCR Investigation
- Methane-loaded (GCR & SPE) Investigation

Introduction

- Fuel cell research focused on hydrogen loading of materials in which the hydrogen can be easily released for use as fuel
  - Space radiation research focused on low-Z materials
  - Can we use a similar concept of loading materials with low-Z substances to increase the radiation mitigation properties of the material?
- 3 classes of materials
  - Metal organic frameworks (MOFs)
  - Metal hydrides (MHs)
  - Nano-porous carbon composites (CNTs)
- Method: HZETRN transport code
  - Tissue detector
  - Output: Dose (cGy)



Previous Work

- Investigated 64 H-loaded materials
- HZETRN 2005 transport code
  - No restrictions on the energy grid for the SPE
- Focused on 19-24, October 1989 Solar Particle Event (SPE)
  - Particularly hard event
- Compared with typical spacecraft material (aluminum) and “gold standard” materials (HDPE)

	MOFs	CNTs	MHs	Total
Dose < HDPE	1	7	1	9
HDPE < Dose < Al	9	7	14	30
Al < Dose	0	0	25	25

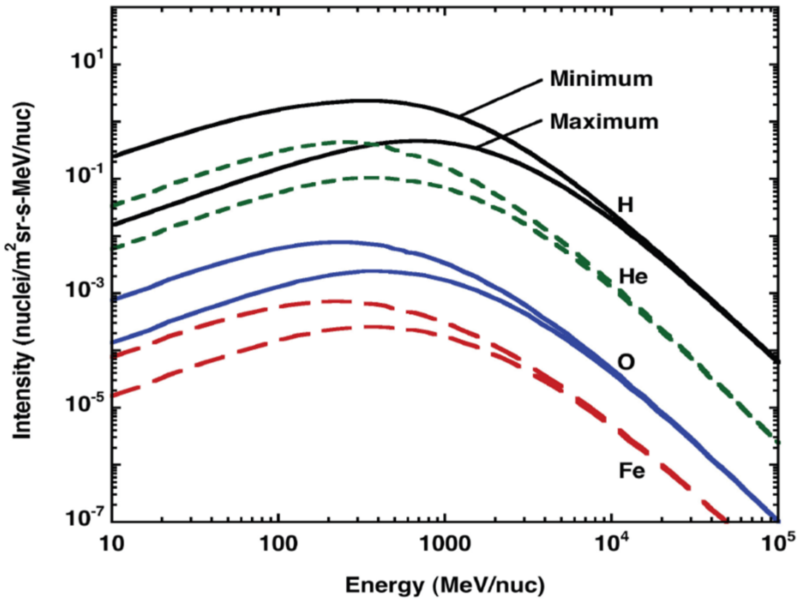
Atwell, W., Rojdev, K., Liang, D., Hill, M., “Select Materials as Space Radiation Shielding Mitigators: Metal Hydrides, MOFs, and Nano-Porous Carbon Composites,” *International Conference on Environmental Systems*, Tucson, July 2014.

Hydrogen-Loaded

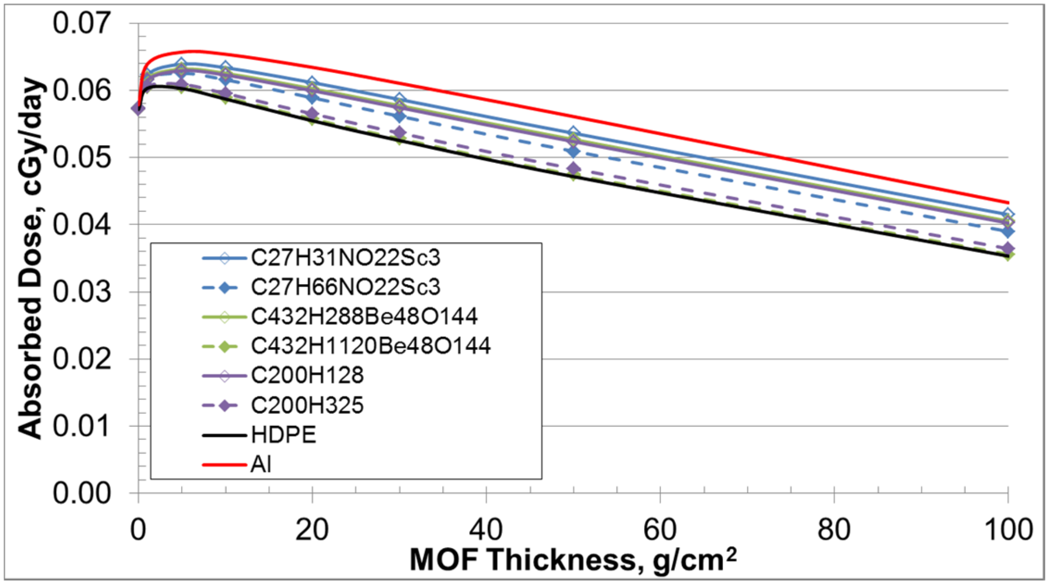
Galactic Cosmic Ray Investigation

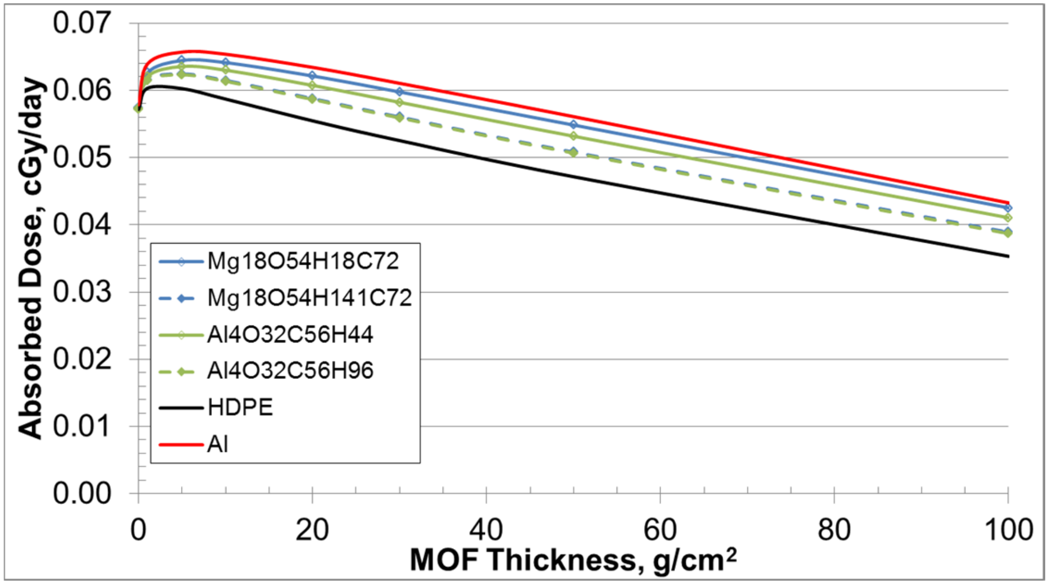
Methods

- 64 materials (same as previous study)
  - 40 metal hydrides (interstitial:26, non-interstitial:7, solution:7)
  - 10 metal organic framework (non-loaded:5, H-loaded:5)
  - 14 carbon composites (non-loaded:7, H-loaded:7)
- Compare with HDPE and Al
- 1977 solar min GCR
- HZETRN 2010



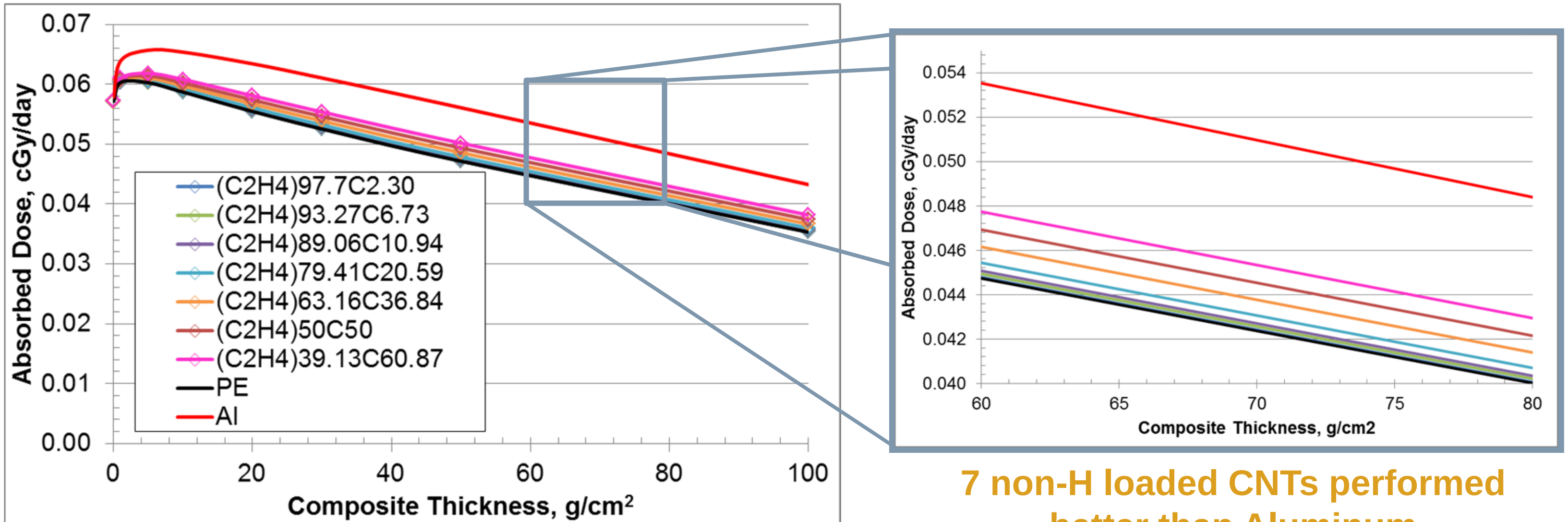
Results: Metal Organic Framework (MOFs)



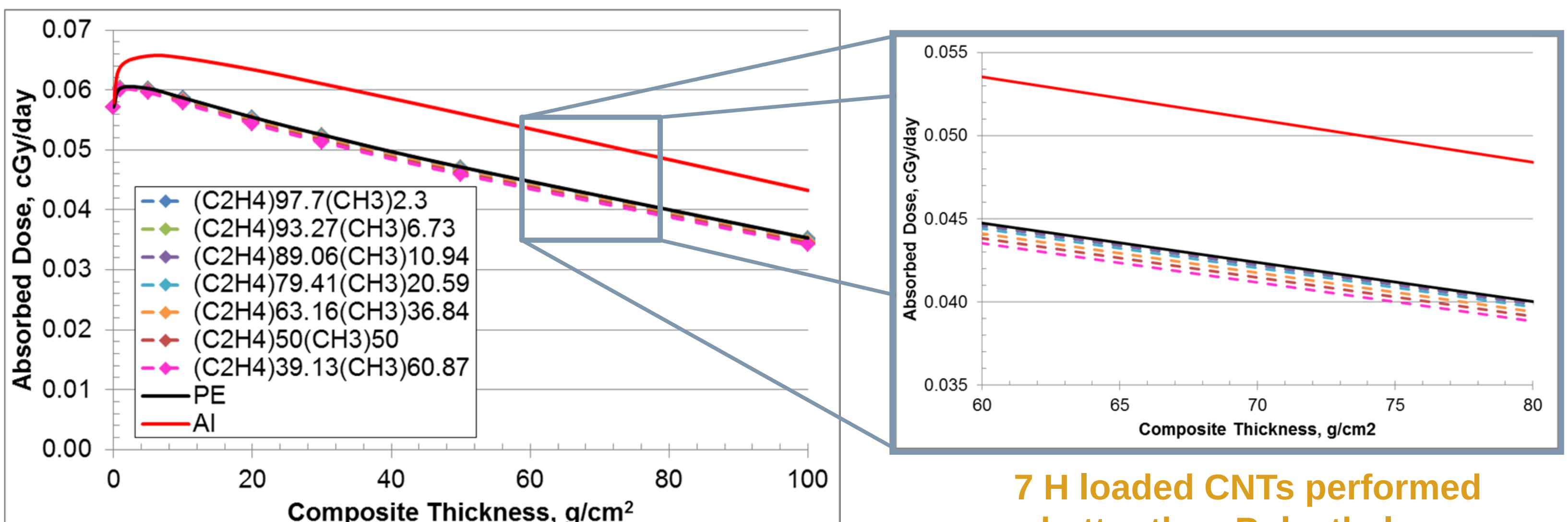


All 10 MOFs performed better than Aluminum

Results: Carbon Composites (CNTs)

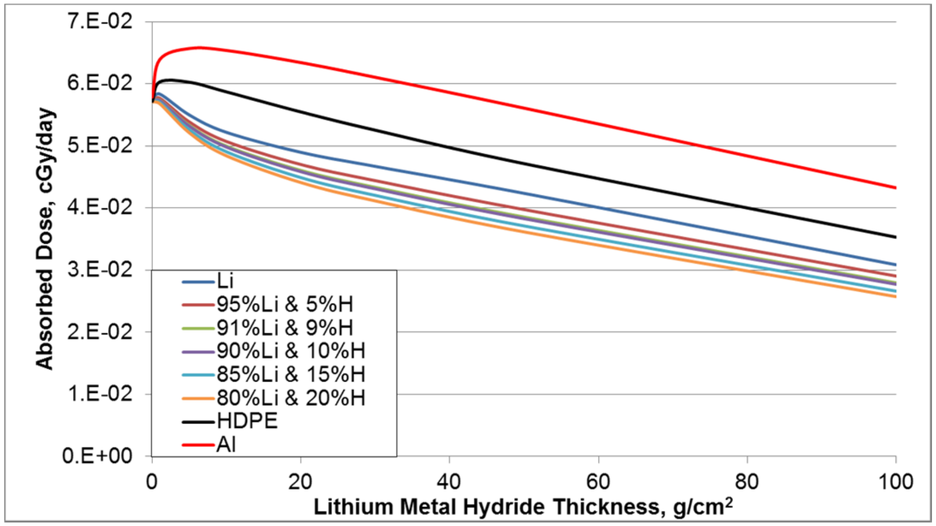


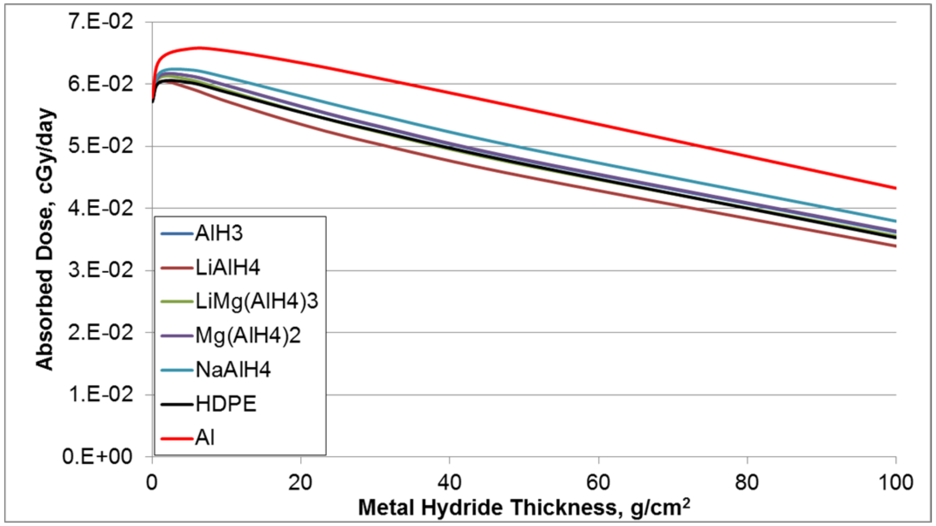
7 non-H loaded CNTs performed better than Aluminum

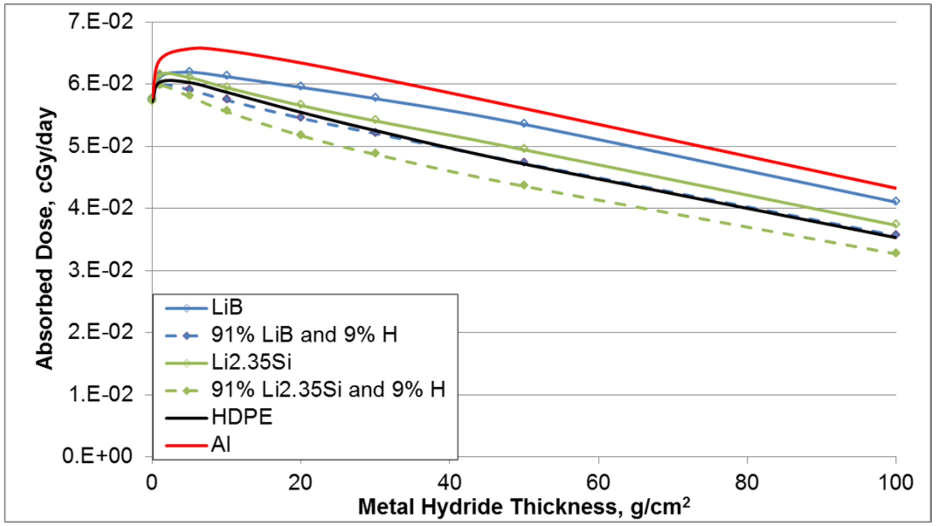


7 H loaded CNTs performed better than Polyethylene

Results: Metal Hydrides







- 9 materials performed better than polyethylene
- 6 materials performed better than aluminum
- 25 materials performed worse than aluminum (not shown in the graphs)

Summary and Recommendations

	MOFs	CNTs	MHs	Total
Dose < HDPE	0	7	9	16
HDPE < Dose < Al	10	7	6	16
Al < Dose	0	0	25	25

- Focus on hydrogenated CNTs
- Focus on lithium metal hydrides

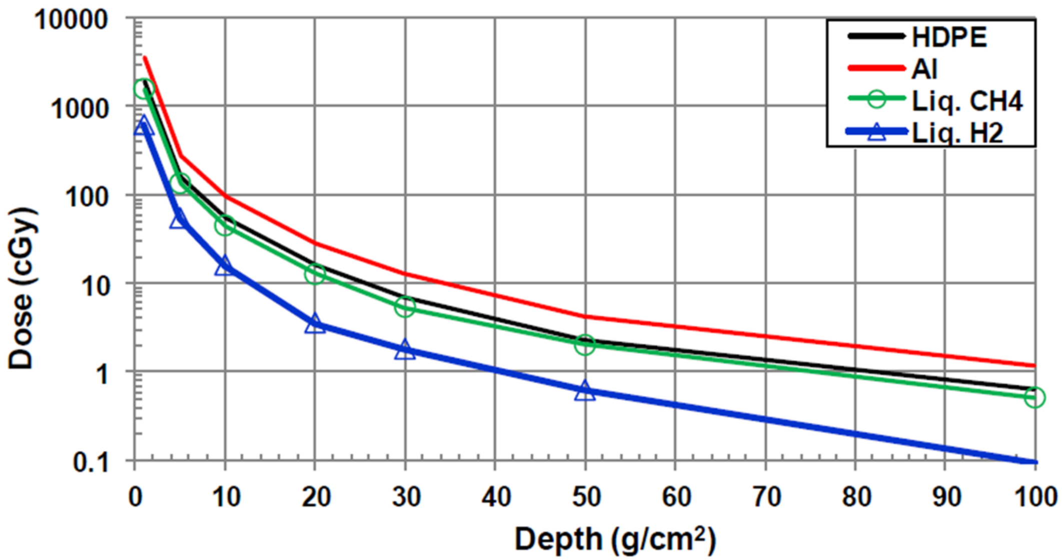
Methane-Loaded

Solar Particle Events

Galactic Cosmic Rays

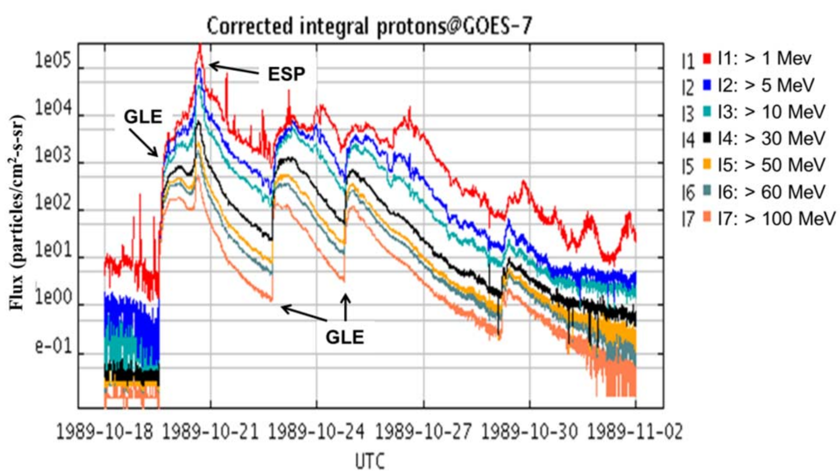
Why Methane?

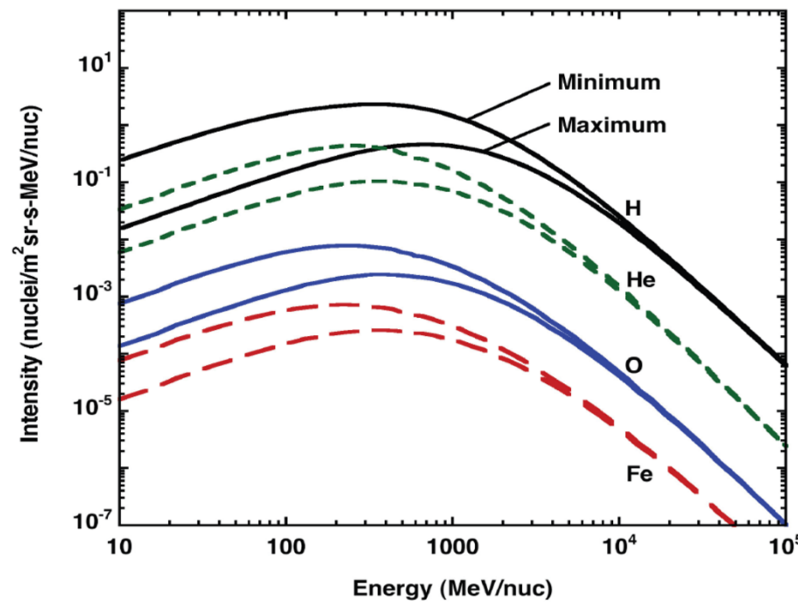
- Problems with hydrogen
  - Stability in changing environmental conditions
  - Safety implications for fires and explosions
- Methane is a slightly better mitigator than HDPE



Methods

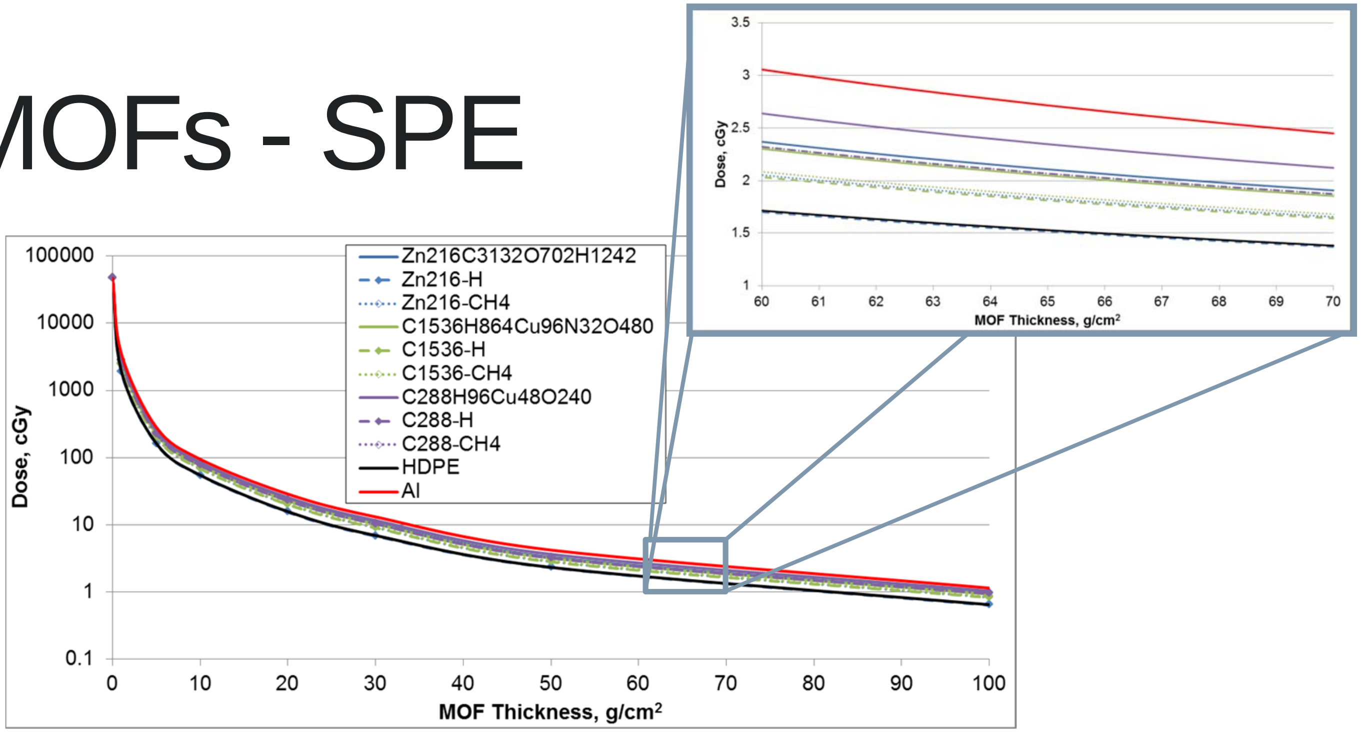
- 36 materials
  - 15 metal organic framework (non-loaded:5, H-loaded: 5, CH_4-loaded:5)
  - 21 carbon composites (non-loaded:7, H-loaded: 7, CH_4-loaded:7)
- Compare with H-loaded versions, HDPE, and Al
- 1977 solar min GCR
- 19-24 October 1989 SPE
- HZETRN 2010

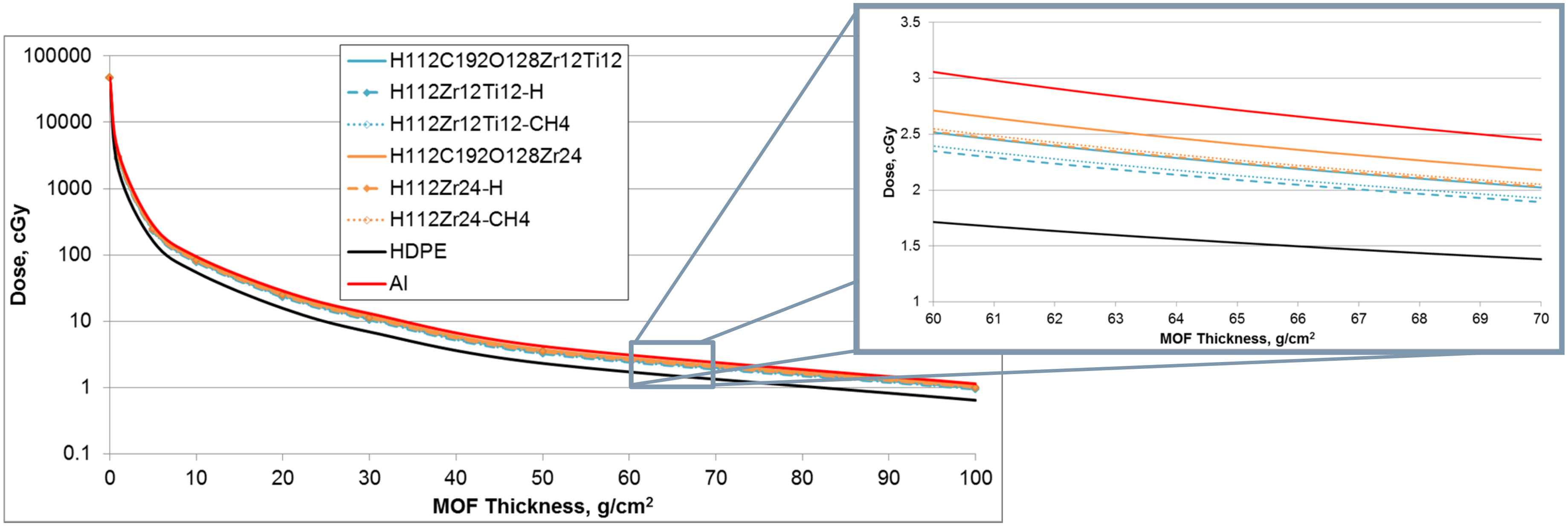




Results: MOFs - SPE

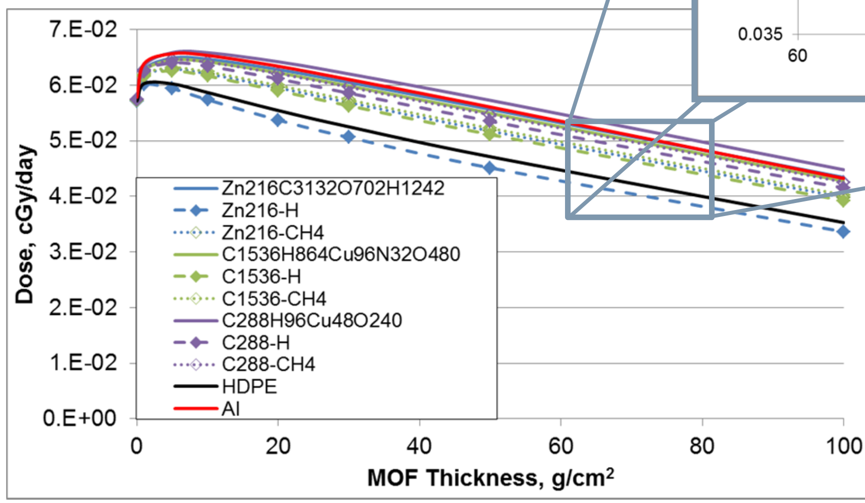
Material (30 g/cm²)	CH4 dose higher than H
Zn216	34%
C1536	3%
C288	0%
H112Zr12Ti12	2%
H112Zr24	1%

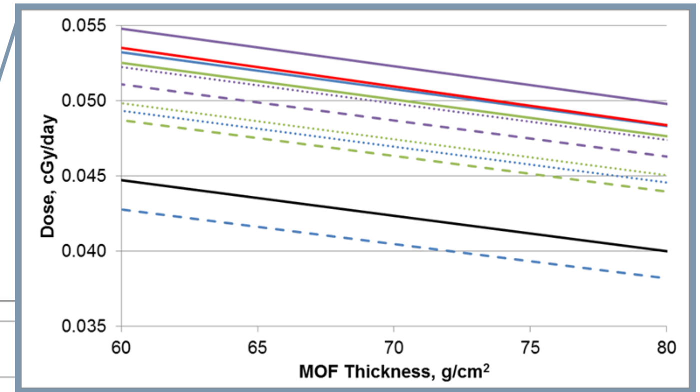


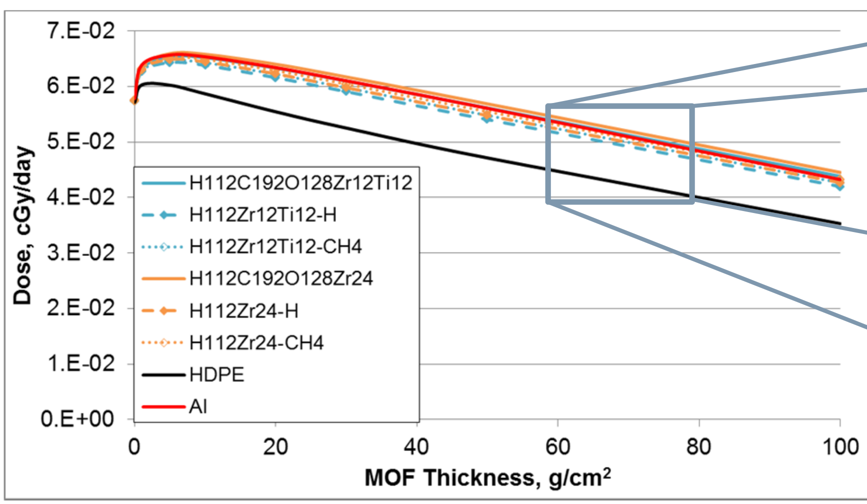


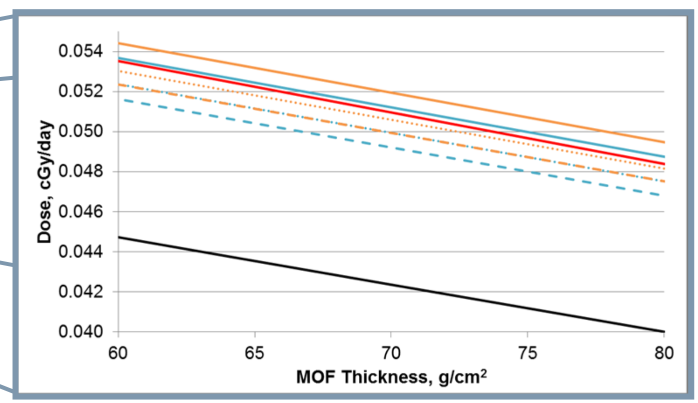
Results: MOFs - GCR

Material (30 g/cm²)	CH4 dose higher than H
Zn216	12%
C1536	2%
C288	2%
H112Zr12Ti12	1%
H112Zr24	1%

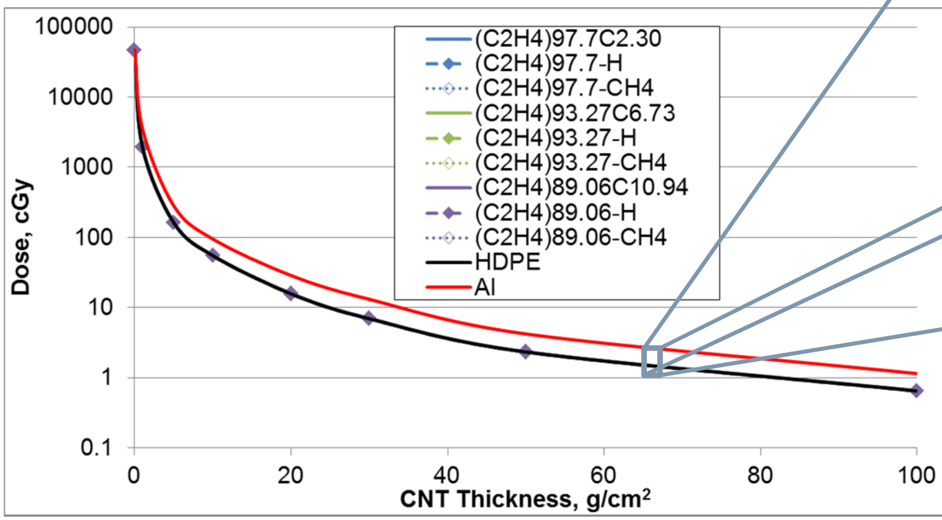


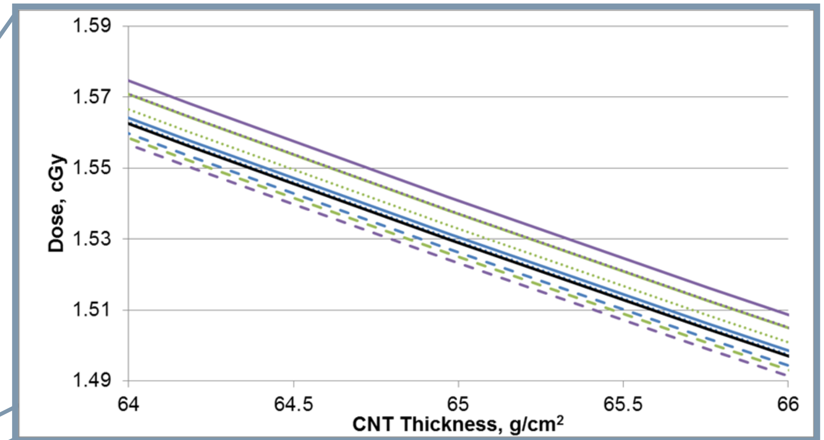






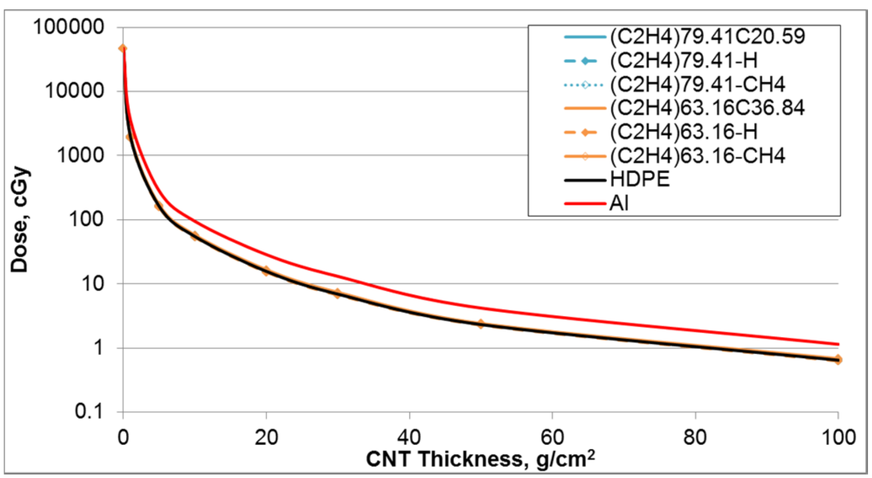
Results: CNTs - SPE

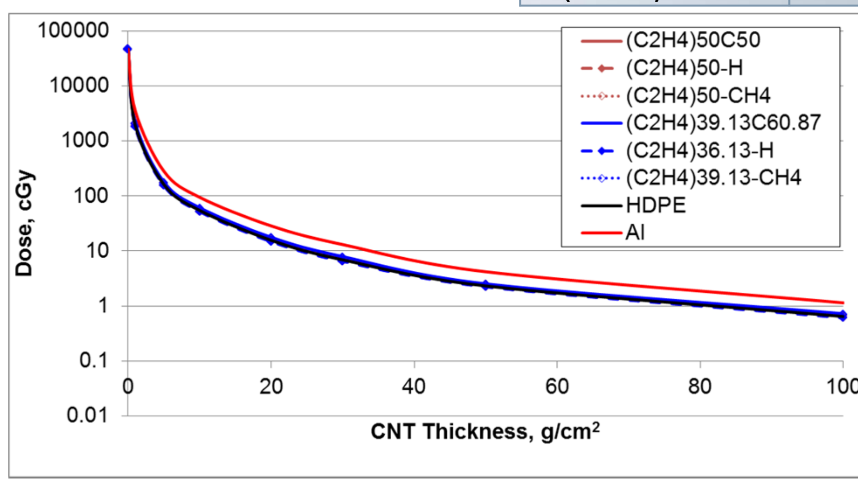




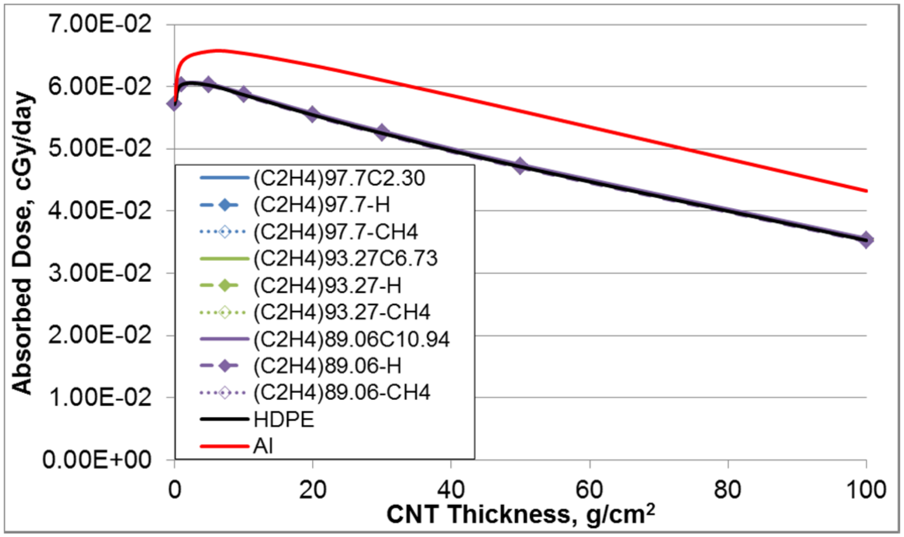
Material (30 g/cm²)	CH4 dose higher than H
(C2H4)97.7	0%
(C2H4)93.27	1%
(C2H4)89.06	2%

Material (30 g/cm²)	CH4 dose higher than H
(C2H4)79.41	4%
(C2H4)63.16	8%
(C2H4)50	12%
(C2H4)39.13	17%

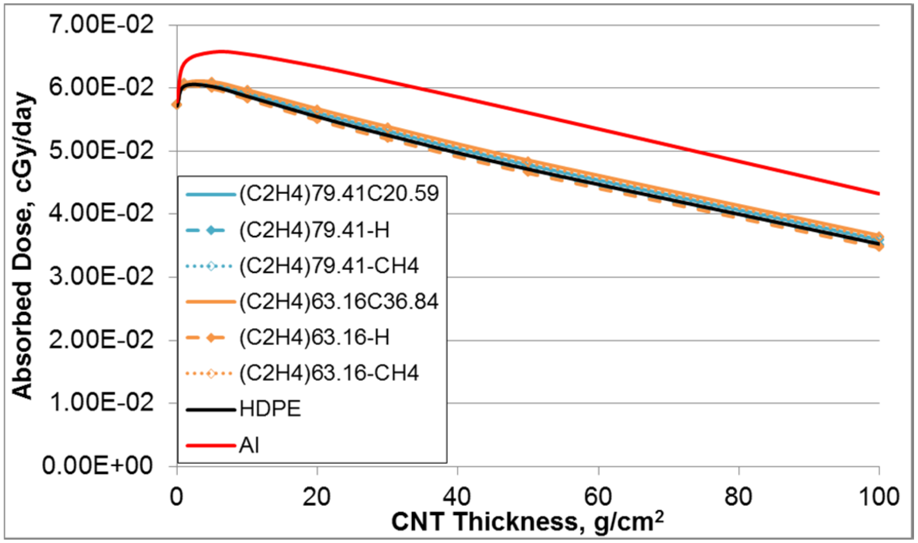


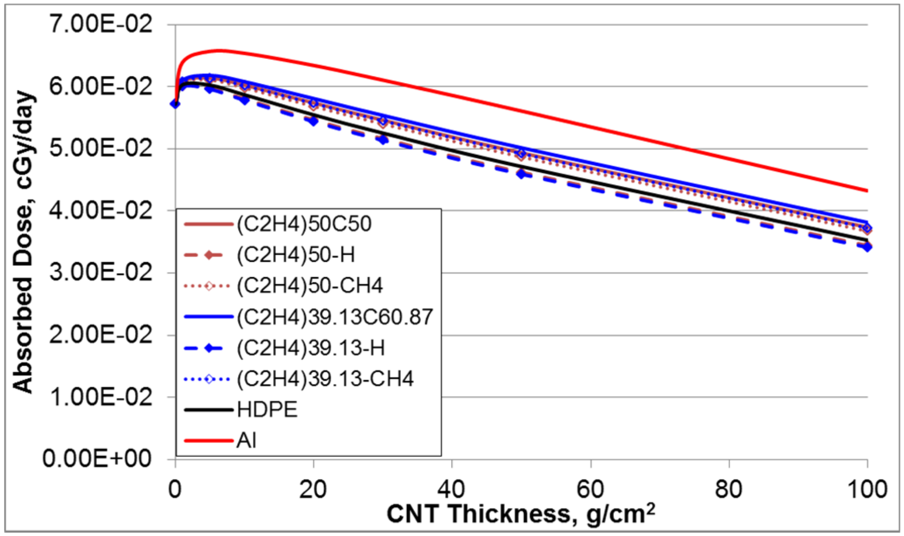


Results: CNTs - GCR



Material (30 g/cm²)	CH4 dose higher than H
(C2H4)97.7	0%
(C2H4)93.27	0%
(C2H4)89.06	1%
(C2H4)79.41	2%
(C2H4)63.16	3%
(C2H4)50	5%
(C2H4)39.13	6%





Summary and Recommendations

- Not much difference in dose between hydrogen and methane loaded materials
    - Concentrate on methane loading to eliminate concerns with hydrogen
- CNTs most promising candidate material

SPE	MOFs	CNTs	Total
Dose < HDPE	1	7	8
HDPE < Dose < Al	14	14	28
Al < Dose	0	0	0

GCR	MOFs	CNTs	Total
Dose < HDPE	1	7	8
HDPE < Dose < Al	11	14	25
Al < Dose	3	0	3

Questions

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BACKUP

Interstitial Metal Hydrides

- New phases after hydrogen loading
- Non-stoichiometric with variable amounts of hydrogen
- Hydrides form via two mechanisms
  - Adsorption of di-hydrogen
  - Electrolytic reduction of ionized hydrogen on the surface, followed by diffusion of protons into the lattice

Formula	Density (g/cm^3)
91% $Li_{2.35}Si$ and 9% H	0.84
91% LiB and 9% H	0.67
96% $CaNi_5$ and 4% H	6.60
96% $LaNi_{4.7}Al_{0.3}$ and 4% H	7.60
96% $LaNi_{4.8}Sn_{0.2}$ and 4% H	8.40
$Ti_{0.98}Zr_{0.02}V_{0.48}Fe_{0.09}Cr_{0.05}Mn_{1.5}$	7.20
$Ti_{0.98}Zr_{0.02}V_{0.48}Fe_{0.09}Cr_{0.05}Mn_{1.5}H_{3.3}$	5.80

Formula	Density (g/cm^3)
Al_2Cu	5.83
Al_2CuH	5.39
AlH_3	2.50
$BaAlH_5$	3.30
$CaNi_5$	6.60
$CaNi_5H_6$	5.01
$LaNi_{4.7}Al_{0.3}$	8.00
$LaNi_{4.7}Al_{0.3}H_6$	6.08
$LaNi_{4.8}Sn_{0.2}$	8.40
$LaNi_{4.8}Sn_{0.2}H_6$	6.38
$LaNi_5$	8.20
$LaNi_5H_6$	6.22
$Li_{2.35}Si$	1.67
LiB	1.65
$SrAl_2H_2$	2.64
$TiCr_{1.8}$	5.70
$TiCr_{1.8}H_{3.5}$	4.50
$TiFe_{0.9}Mn_{0.1}$	6.50
$TiFe_{0.9}Mn_{0.1}H_2$	5.20

Non-Interstitial and Solution Metal Hydrides

- Non-interstitial
  - Expanded lattice after hydrogen loading
  - Not transformed into new structure
- Solution
  - Do not have transformed crystal structures post-hydrogen loading

Solution Formula	Density (g/cm^3)
80% Li and 20% H	0.57
85% Li and 15% H	0.56
90% Li and 10% H	0.55
91% Li and 9% H	0.82
95% Li and 5% H	0.54
Li	0.53
V	6.00

Non-Interstitial Formula	Density (g/cm^3)
$LiAlH_4$	0.92
$LiMg(AlH_4)_3$	1.80
$Mg(AlH_4)_2$	2.24
$NaAlH_4$	1.81
VH	5.60
VH_2	2.30
$Y_3Al_2H_{6.5}$	4.10

Metal Organic Frameworks (MOFs)

- Two components to MOFs
  - Metal ion or cluster of metal ions
  - Organic molecule (i.e. linker)
    - Mono-, di-, tri-, or tetravalent ligands

Hydrogen Loaded Formula	Density (g/cm³)
$Zn_{216}\ C_{3132}\ O_{702}\ H_{14813.5}$	0.2996
$C_{432}\ H_{1120}\ Be_{48}\ O_{144}$	0.460
$Mg_{18}\ O_{54}\ H_{141}\ C_{72}$	0.953
$Al_{4}\ O_{32}\ C_{56}\ H_{96}$	1.680
$C_{200}\ H_{325}$	0.3522

Non-Hydrogen Loaded Formula	Density (g/cm³)
$Zn_{216}\ C_{3132}\ O_{702}\ H_{1242}$	0.247
$C_{432}\ H_{288}\ Be_{48}\ O_{144}$	0.423276
$Mg_{18}\ O_{54}\ H_{18}\ C_{72}$	0.905589
$Al_{4}\ O_{32}\ C_{56}\ H_{44}$	1.610
$C_{200}\ H_{128}$	0.314945

Nano-Porous Carbon Composites (CNTs)

Non-Hydrogen Loaded Formula	Density (g/cm^3)
$(C_2H_4)_{97.7}\,C_{2.30}$	0.95
$(C_2H_4)_{93.27}\,C_{6.73}$	0.96
$(C_2H_4)_{89.06}\,C_{10.94}$	0.97
$(C_2H_4)_{79.41}\,C_{20.59}$	1.00
$(C_2H_4)_{63.16}\,C_{36.84}$	1.04
$(C_2H_4)_{50}\,C_{50}$	1.10
$(C_2H_4)_{39.13}\,C_{60.87}$	1.16

Hydrogen Loaded Formula	Density (g/cm^3)
$(C_2H_4)_{97.7}\,(CH_3)_{2.3}$	0.95018
$(C_2H_4)_{93.27}\,(CH_3)_{6.73}$	0.96054
$(C_2H_4)_{89.06}\,(CH_3)_{10.94}$	0.9709
$(C_2H_4)_{79.41}\,(CH_3)_{20.59}$	1.0018
$(C_2H_4)_{63.16}\,(CH_3)_{36.84}$	1.0436
$(C_2H_4)_{50}\,(CH_3)_{50}$	1.1054
$(C_2H_4)_{39.13}\,(CH_3)_{60.87}$	1.1672